

organic liquids. New measurements of Pb(II) sorption on powdered corundum indicate sorption of polymeric species, suggesting that substrate structure is influencing the surface Pb(II) complexation. Comparative studies of the role of organic complexation on the sorption of Cu(II) on the surface of amorphous SiO₂ and on powdered corundum are aimed at specifying surface complexation mechanisms.

Keywords: Surface Complexation, Interface Reactions, Synchrotron X-ray Absorption Spectroscopy

DIVISION OF ADVANCED ENERGY PROJECTS

The Division of Advanced Energy Projects (AEP) provides support to explore the feasibility of novel, energy-related concepts that evolve from advances in basic research. These concepts are typically at an early stage of scientific development and, therefore, are premature for consideration by applied research or technology development programs. The AEP also supports high-risk, exploratory concepts that do not readily fit into a program area but could lead to applications that may span several disciplines or technical areas.

The Division provides a mechanism for exploring the conversion of basic research results into applications that could impact the Nation's energy economy. AEP does not support ongoing, evolutionary research or large scale demonstration projects. Technical topics include physical, chemical, materials, engineering, and biotechnologies. Projects can involve interdisciplinary approaches to solve energy-related problems. The DOE Contact for this program is Walter M. Polansky, (301) 903-5995.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

190. COMBUSTION SYNTHESIS AND ENGINEERING OF NANOPARTICLES FOR ELECTRONIC, STRUCTURAL AND SUPERCONDUCTOR APPLICATIONS

\$196,000

DOE Contact: Walter M. Polansky, (301) 903-5995

Alfred University Contact: Gregory C. Stangle,
(607) 871-2798

The investigation will: (1) produce nanoparticles of multicomponent oxide ceramic materials by a combustion synthesis technique that is readily scaled up; (2) apply proven, in-house grain-boundary engineering methods to fine-tune microstructure evolution during densification; (3) use conventional and rapid sintering techniques to

densify consolidated nanoparticle compacts; and (4) characterize the material at each stage. Expected results include: (a) the synthesis of nanoparticles of complex composition for use in several applications (such as YBa₂Cu₃O_{7-x}, a high-temperature superconductor with uses, e.g., in magnetic flux trapping and high-speed capacitor applications; yttria-stabilized zirconia for, e.g., high surface toughness materials for high-temperature applications; and BaTiO₃, a material expected to possess superparaelectric properties when nanocrystalline); (b) the development and reduction to practice of a generic, widely applicable process; and (c) the evaluation of the energy efficiency and commercialization potential of the process. The proposed study will enlist three U.S.-based companies to aid in focusing the research toward the commercialization of successful research results.

Keywords: Nanoparticles, Ceramics, Superconductors, Electronic Materials

191. CREATION AND DESTRUCTION OF C₆₀ AND OTHER FULLERENE SOLIDS

\$302,000

DOE Contact: Dr. Walter M. Polansky, (301) 903-5995

University of Arizona Contact: Donald R. Huffman,
(602) 621-4804

This work will focus on the creation and destruction of fullerenes to produce new materials of interest to the Department of Energy. It is now known that, besides the famous C₆₀ molecule (buckminsterfullerene), hundreds of other fullerenes, with masses of up to 600 carbon atoms, are also synthesized in the Krätschmer-Huffman process. The physics underlying the creation of the fullerenes is poorly understood and the major portion of this work will be a systematic study of the process. This will involve construction of a new, fully-instrumented smoke-chamber, that will be used in a methodical exploration of fullerene yield versus production conditions. Recent reports of the successful seeding of chemical vapor deposition (CVD)-grown diamond films using thin films of C₇₀ and of the room-temperature conversion of solid C₆₀ into diamond powder via non-hydrostatic compression, indicate that some of the first important commercial applications of the fullerenes may involve their destruction as a means of synthesizing high-performance materials. This work will include a systematic study of the destruction and modification of the various fullerenes by chemical reaction, electromagnetic radiation, and electron bombardment.

Keywords: Fullerenes, Diamond Powders, Buckyballs

192. SYNTHESIS AND PROPERTIES OF HIGH STRENGTH NANOLAYERED COMPOSITES

\$330,000

DOE Contact: Walter M. Polansky, (301) 903-5995
Los Alamos National Laboratory Contact:
Michael Nastasi, (505) 667-7007

The objective of this project is to synthesize and evaluate ultra high strength vapor-deposited nanoscale materials both in the monolithic and composite form. Such materials have been shown to possess strengths that are within a factor of three or four of the theoretical shear strength $\approx \mu/15$, where μ is the shear modulus. Synthesis of nanoscale materials presents the opportunity to develop a basic understanding of the deformation and fracture mechanisms that operate close to the theoretical limit of strength of materials to enable a new technological breakthrough, namely mechanical miniaturization. The availability of the fine-scale ultra high strength materials would provide the basis for fabricating, among others, miniature activators, springs, and diaphragms, for biomedical or sensor applications. The primary performance task will be to synthesize ductile materials with ultra high strength for application in mechanical miniaturization.

Keywords: Nanostructures, Composites, Mechanical Miniaturization

193. OPTIMALLY CONTROLLED INTERIOR MANIPULATION OF SOLIDS

\$299,000

DOE Contact: Walter M. Polansky, (301) 903-5995
Princeton University Contact: Herschel Rabitz,
(609) 258-3917

This project is concerned with the development of a technique for modification of the interior solids without the necessity of opening up the material. The technique is based on the concept of designing and creating temporally and spatially tailored laser pulses that deposit energy on the surface for the purpose of launching an intense acoustic wave that focuses within the solid. Taking account of the relatively large illumination area on the surface and the focusing nature of the acoustic waves, it should be possible to minimally disrupt the surface while still attaining significant degrees of interior modification at the target volume. A central feature of this new materials processing method is its reliance on destructive and constructive interference between the ensuing shear and compressional acoustic waves. The research will include a theoretical design component. An established capability for interior manipulation of solids would open up many opportunities including interior annealing, induced phase

transitions, induced chemical reactions, crack arresting, controlled defect site generation, and interior welding.

Keywords: Interior Processing of Materials, Acoustic Manipulation

194. PHOTOREFRACTIVE LIQUID CRYSTALS: NEW MATERIALS FOR ENERGY-EFFICIENT IMAGING TECHNOLOGY

\$320,000

DOE Contact: Walter M. Polansky, (301) 903-5995
Argonne National Laboratory Contact:
Gary P. Wiederrecht, (708) 252-6963

This project will develop a new class of materials that will be used to produce energy-efficient image processing micro-devices. These materials will exploit the photorefractive effect, a light-induced change in the refractive index of a nonlinear optical materials that results from photogeneration of a space charge field caused by directional charge transport over macroscopic distances within a solid. Both frequency and phase information contained in light that has passed through a distorting medium can be recovered noise-free using photorefractive materials. The only high quality photorefractive materials commercially available today are expensive single crystals of inorganic materials such as barium titanate. This project will develop a completely new approach that combines cheap, easily processed organic materials with a built-in method of achieving the solid state order necessary to achieve photorefractivity comparable to that seen in inorganic crystals. The new approach uses organic molecules that undergo a phase transition above ambient temperatures to a liquid crystalline phase. These thin solid films have the potential to possess greater photorefractive sensitivity and faster responses times than any material developed to date.

Keywords: Photorefractive Liquid Crystals, Image Processing, Nonlinear Optical Materials

195. RAPID MELT AND RESOLIDIFICATION OF SURFACE LAYERS USING INTENSE, PULSED ION BEAMS

\$300,000

DOE Contact: Walter M. Polansky, (301) 903-5995
Sandia National Laboratories Contact:
Regan W. Stinnett, (505) 845-7488

This project will develop a surface processing technology based on new, repetitively pulsed ion beams. Rapid solidification is known to greatly improve metal surface properties such as corrosion, wear, and fatigue resistance, but the lack of an economic and effective way to apply this technique to surfaces has prevented its use except in high value applications. Intense, pulsed, high energy ion beams

treat surfaces to produce non-equilibrium microstructures, nanocrystalline phases, and extended solid solutions leading to improved corrosion and friction properties of metals, as well as surface smoothing and defect healing, grain refinement, and modification of surface layer hardness. The low cost and in-depth deposition of high energy pulsed ion beams gives pulsed ion beam technology important advantages over laser treatment. The project will determine the capabilities and limitations of rapid melt and resolidification using pulsed ion beams. It will document the non-equilibrium micro-structures produced in treated layers and their effect on metal surface properties and will do the initial process development needed to show how this technique can be applied to commonly used metals. If successful, this will enable new ways to modify surfaces for enhanced properties and lifetimes with greatly improved energy efficiency and cost-effectiveness and will enable a significant reduction in the use of heavy metal and solvent-based surface treatment coating processes.

Keywords: Surface Processing, Pulsed Ion Beams, Rapid Solidification

196. 'OFF DIAGONAL' THERMOELECTRICITY FOR COOLING AND POWER GENERATION
\$170,000

DOE Contact: Walter M. Polansky, (301) 903-5995
TecOne Contact: Louis R. Testardi, (904) 562-9789

'Off-Diagonal' thermoelectricity, an uncommon effect which only occurs in low symmetry materials, allows unique and untried opportunities for thermal cooling, heat pumping and power generation. It utilizes the orthogonal coupling of heat and electric current flows in anisotropic media and opens new device as well as material development routes for the improvement of thermoelectric energy conversion. The advantages lie in a geometry naturally adapted to compact cooling, heat pumping and power generation with planar thermal boundaries, and also in electric impedances which allow a more compact, efficient and convenient device. The overall program goal is the development of lightweight, flexible sheet materials which will provide cooling, heat pumping and, with less application, power generation for objects or temperature baths of irregular geometry using 'off-diagonal' thermoelectricity. The principal materials thrust will be in conducting polymers because of their potential low cost and their ease of large scale processing to develop anisotropic properties. Applications include cooling of small volume consumer/industrial items, cooling and temperature control

of the human body for medical treatment and comfort, and the utilization of waste heat from large area temperature baths.

Keywords: Off-Diagonal Thermoelectricity, Thermal Cooling, Thermal Heating

197. EVAPORATION THROUGH TUNGSTEN TO ACHIEVE HIGH-RATE VAPOR PHASE PROCESSING OF INTERMETALLICS

\$291,000

DOE Contact: Walter M. Polansky, (301) 903-5995
General Electric Company Contact: David W. Skelly, (518) 387-6534

Modification of current practice of electron beam processes has been found to enhance chemistry uniformity and deposition rates through the addition of tungsten to the evaporation pool to permit much higher pool temperatures and stable pool dynamics. The objective of this research is to define optimum operating conditions for achieving economic deposition of controlled-chemistry, controlled-thickness Ni-base superalloys, NbTi-base metallic materials, and high strength, high temperature intermetallic phases. The approach will be to: evaluate process stability during prolonged evaporation through a tungsten-rich liquid pool; measure the effect of tungsten concentration in the pool on the evaporation process; characterize the influence of electron beam scan rate and scan pattern on the deposit chemistry and deposition rate; characterize the influence of the source temperature profile on deposit chemistry and deposition rate; determine evaporation conditions for Ni-base alloys containing Ta and Mo; and extend the electron beam evaporation-through-tungsten processing to higher melting intermetallic phases and NbTi-base metals. The understanding derived from this investigation will have significant impact on the ability to fabricate advanced designs of turbine blades.

Keywords: Superalloys, Intermetallics, Electron Beam Processing, Turbine Blades

198. ULTRASONIC AND DIELECTRIC NONINVASIVE DIAGNOSTICS FOR SINTERING OF CERAMIC COMPOSITES

\$342,000

DOE Contact: Walter M. Polansky, (301) 903-5995
Johns Hopkins University Contact: Moshe Rosen, (410) 516-8678

The potential advantages of using microwaves to process ceramics have been recognized for more than three decades. However, a profound understanding of how

materials interact with microwaves during sintering is still lacking. Measurement of the dielectric and mechanical properties of a material during microwave processing in real-time can provide the necessary theoretical and experimental insight into understanding this interaction that can subsequently be applied for the optimization of microwave processing of materials. In the course of this project, *in situ*, nonintrusive diagnostics for microwave sintering of ceramic materials will be developed. The essence of the project is a specially designed system for ultrasonic and dielectric probes to be integrated within the microwave furnace. The ultrasonic data can be ultimately related to the densification process during sintering of ceramics, while the dielectric characteristics are connected to the absorption mechanism of the microwave energy by the ceramic material. Acquisition of such data during sintering will shed light on the sintering kinetics and its mechanism and, consequently, provide an understanding of the optimal sintering conditions needed to achieve maximum densification and the desired material properties.

Keywords: Microwave Sintering, Ceramics, Noninvasive Diagnostics

199. COMPACT MEV ION IMPLANTER

\$319,000

DOE Contact: Walter M. Polansky, (301) 903-5995
Lawrence Berkeley Laboratory Contact:
Simone Anders, (510) 486-6745

A new kind of MeV ion implanter will be developed, the distinguishing features of which will be its relatively small size and low cost. The heart of the device will be a novel kind of ion source by means of which high charge state ions will be produced, thereby allowing the production of high energy ion beams (1 MeV and above), using only modest accelerating voltages (one to several hundred kV). The ion source will be a repetitively pulsed vacuum spark source, and the implantation facility will thus also generate repetitively pulsed, large area, metal ion beams. By virtue of the relatively low voltages employed the implanter will be much more compact and of much lower cost than present state-of-the-art facilities that employ singly charged ions and megavolt power supplies. From the perspective of new physics, a novel kind of ion source will be developed. Vacuum arc ion sources have been developed but not vacuum spark ion sources, and it is in the latter that the highly stripped ions are to be found, yielding high energy at modest voltage. From the perspective of new technology, this is an entirely new approach to doing MeV ion implantation, making high energy surface modification techniques feasible for a vastly broader field of users than at present.

Keywords: Ion Source, Ion Implanter, Ion Beams, Surface Treatment

200. THERMOELECTRIC QUANTUM WELLS

\$350,000

DOE Contact: Walter M. Polansky, (301) 903-5995
Lawrence Livermore National Laboratory Contact:
Joseph C. Farmer, (510) 423-6574

Solid state thermoelectric devices have no moving parts and can be used to convert heat directly into electricity. Such devices can also be used as chlorofluorocarbon (CFC)-free refrigerators, provided that an external voltage is applied. Unfortunately, thermoelectric devices are not as efficient as their mechanical counterparts. However, theoretical physicists at the Massachusetts Institute of Technology have recently used quantum mechanics to design a new class of thermoelectric materials that may improve the efficiency (figure of merit) of thermoelectric devices to a point where they are competitive with conventional internal combustion engines and CFC-based refrigerators. Process technology developed at Lawrence Livermore National Laboratory for the fabrication of X-ray optics is now being used to synthesize these new multilayer thermoelectric thin films. Multilayers are being made by alternately sputtering quantum well and barrier layers onto a moving substrate from dual magnetrons. A number of multilayer films, including high-temperature $\text{Si}_{0.8}\text{Ge}_{0.2}/\text{Si}$ and low-temperature $\text{Bi}_{0.9}\text{Sb}_{0.1}/\text{PbTe}_{0.8}\text{Se}_{0.2}$, are being synthesized and evaluated. This research can lead to new materials and devices.

Keywords: Quantum Wells, Thermoelectric Devices

201. POROUS CARBONS: CONTROLLING STRUCTURE, COMPOSITION AND PERFORMANCE

\$355,000

DOE Contact: Walter M. Polansky, (301) 903-5995
Lawrence Livermore National Laboratory Contact:
Richard W. Pekala, (510) 422-0152

This research examines the synthesis and processing conditions necessary to tailor the local structure and composition of porous carbons for potential applications in energy storage devices. Carbon aerogels are being formed from resorcinol-formaldehyde and phenolic-furfural precursors. These porous carbons have low electrical resistivity, an ultrafine pore size distribution, high surface area (400 to 1100 square meters per gram, roughly the size of one or two basketball courts), and a solid matrix composed of interconnected particles or fibers. Preliminary data show that these materials are attractive electrodes for double layer capacitors. The project investigates sol-gel polymerization of multifunctional organic monomers, the phase separation of polymer/solvent mixtures, the formation of porous composites, intrinsic chemical doping, and pyrolysis in controlled atmospheres. A variety of characterization tools are being used to study the structure

and properties of porous carbons. The overall objective is to develop a fundamental understanding of how morphology, chemical composition, and local order affect the electrochemical performance of porous carbons. The potential payoff from this research is the development of new energy storage devices with superior performance.

Keywords: Porous Carbons, Energy Storage Devices

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

202. FEASIBILITY OF A NOVEL APPROACH FOR FAST, ECONOMICAL DETERMINATION OF RADIATION DAMAGE IN NUCLEAR REACTOR CORES

\$149,000

DOE Contact: Walter M. Polansky, (301) 903-5995

University of Michigan Contact: Gary S. Was,
(313) 763-4675

The objective of this project is to determine the feasibility of using proton irradiation as a radiation damage tool, resulting in order-of-magnitude savings in time and cost over current methods to study radiation damage. The feasibility will be established through the application of proton irradiation to the determination of the mechanism of irradiation assisted stress corrosion cracking (IASCC) in light water reactors (LWRs). The emphasis of the technical program will be on the role of grain boundary chemistry and microstructural changes on IASCC. High energy proton irradiation has recently been shown to produce grain boundary segregation of the major alloying elements and impurities, and a microstructure that is comparable to that produced by neutron irradiation in a fraction of the time and at a fraction of the cost. This program is designed to uncover the effects of grain boundary impurity segregation, chromium depletion, and the irradiated microstructure on IASCC. It involves both experimental and computational efforts. The plan also calls for investigation of the dose, dose rate, temperature and injected hydrogen effects and comparison with available neutron irradiation data.

Keywords: Radiation Damage, Stress Corrosion Cracking, Irradiated Microstructures

203. HOT CARRIER SOLAR CELLS

\$330,000

DOE Contact: Walter M. Polansky, (301) 903-5995

National Renewable Energy Laboratory Contact:
Mark C. Hanna, (303) 384-6620

This project is focused on the development and understanding of a new kind of high efficiency solar cell, called a Hot Carrier Solar Cell (HCSC), which may have the potential

to double the maximum efficiency of conventional solar cells. The ultimate thermodynamic conversion efficiency of an optimized HCSC is 66 percent, compared to 31 percent for an optimized conventional single bandgap solar cell. This project will attempt to utilize the excess kinetic energy of higher energy (hot) carriers generated by the absorption of high energy photons in the solar spectrum, which is normally unavailable for useful work. The HCSC employs a new superlattice structure to absorb the solar photons and to inhibit hot carriers from cooling in the photovoltaic device. Hot carriers from the superlattice region are collected in high bandgap contacts to produce a higher photovoltage. With this combination, the photocurrent and photovoltage of the cell can be separately controlled and optimized. This project will synthesize HCSCs, measure their performance and properties, compare them to appropriate conventional solar cells, and develop a theoretical model for predicting the device characteristics of the HCSC.

Keywords: Hot Carrier Solar Cells, High Efficiency Energy Conversion

204. ATOMIC AND NANOSCALE ENGINEERING OF THERMOPHOTOVOLTAIC SEMICONDUCTORS USING SCANNING PROBE MICROSCOPY TECHNIQUES

\$552,000

DOE Contact: Walter M. Polansky, (301) 903-5995

National Renewable Energy Laboratory Contact:
Lawrence L. Kazmerski, (303) 275-3711

This project uses scanning probe microscopies for the atomic-scale engineering of semiconductors leading to advances in understanding their improvement, and their use in energy-conversion thermophotovoltaic (TPV) structures and devices. This project consists of three interrelated segments: (1) preparation of selected GaInAs and GaInAsP alloy surfaces having suitable compositions; (2) use of modern electronic structure theory to predict the properties of these semiconductor surfaces before and after atomic-scale engineering takes place and to provide guidance for the experiments; and the central and primary activity, (3) evolution of the novel atomic processing microscope to image, process (including atom removal and placement), and characterize these semiconductors with the same nanoscale spatial resolutions and to produce nanometer-scale optimized TPV structures for the next generation of these energy conversion devices.

Keywords: Thermophotovoltaics, Atomic Force Microscopy

205. FABRICATION AND CHARACTERIZATION OF MICRON SCALE FERROMAGNETIC FEATURES
\$133,000

DOE Contact: Walter M. Polansky, (301) 903-5995
University of Nebraska Contact: Peter A. Dowben,
(402) 472-9838

This is a project to study micro scale features of ferromagnetic nickel, cobalt, cobalt-palladium alloys and cobalt-palladium heterostructures fabricated by "direct writing," i.e., by selective area deposition from organometallic compounds. Two goals for this research program are: (1) making magnetic features smaller and smaller, in a variety of different shapes to elucidate the influence of defects on magnetization reversal and coercivity; (2) the project will determine if there is any coupling between small ferromagnetic features (approximately 1 micron), possibly substrate mediated, on the length scale of 1000 angstroms smaller. Polarized light microscopy will be used to image micron scale features and coercivity. A microscope will be used to make polar Kerr rotation measures and obtain spatially selective magnetic information. Spin polarized inverse photoemission with both longitudinal and transverse spin polarization will also be used for probing electronic structures. A new technique for fabricating micro-scale ferromagnetic features involves organometallic chemical vapor deposition techniques to deposit pure metal features with excellent spatial resolution, developed at this laboratory. These techniques allow selective deposition of features as small as 0.2 microns, and as thin as a few monolayers or as thick as 10 microns. The approach is superior to techniques employing ion beams or conventional lithography and is inexpensive and compatible with the fabrication of the next generation of optical and magnetic recording media.

Keywords: Ferromagnetic Features, Micron-Scale Magnets, Organometallic CVD

206. PHOTOCHEMICAL SOLAR CELLS
\$150,000

DOE Contact: Walter M. Polansky, (301) 903-5995
National Renewable Energy Laboratory Contact:
Arthur J. Nozik, (303) 384-6603

Very high power conversion efficiencies (8-12 percent) for photochemical solar cells were reported in 1991. These solar cells consist of highly porous nanocrystalline films of TiO₂ (band gap=3.0 eV) that are sensitized to the visible region of the solar spectrum through adsorption of Ru-containing metal-organic dye complexes on the TiO₂ particle surface. This represents more than two orders of magnitude improvement in the power conversion efficiency of dye-sensitized semiconductor electrodes in a

photochemical cell. A dye-sensitized photochemical solar cell system based on TiO₂ powders could yield low cost and high semiconductor photostability. This project is an integrated program of basic and applied development research that is funded jointly by three U.S. Department of Energy program offices: the Division of Chemical Sciences in the Office of Basic Energy Sciences, the Photovoltaic program in the Office of Utility Technology and Advanced Energy Projects. Research is also occurring to study other organic heterojunctions with wide bandgap semiconductors for photovoltaic applications. The AEP portion of the project is to develop a configuration where the system is able to efficiently split water into hydrogen and oxygen, rather than to produce electricity. An inexpensive source of solar-produced hydrogen would be greatly beneficial to the energy economy of the world, and would result in the use of hydrogen as a non-polluting substitute for many of the fuels currently in use.

Keywords: Photochemical Solar Cells, Hydrogen Production, Dye-Sensitive Semiconductors

207. SEMICONDUCTOR BROADBAND LIGHT EMITTERS
\$330,000

DOE Contact: Walter M. Polansky, (301) 903-5995
Sandia National Laboratories Contact: Paul Gourley,
(505) 844-5806

Semiconductors are compact, lightweight, operate in air, and are rugged. However, conventional semiconductor diodes emit light only into a narrow range of wavelengths. To obtain broadband emission, new structures are needed that utilize a wide range of alloy compositions available from modern semiconductor growth techniques. Fractal lattice and chirped quantum wells form a new class of materials which can provide broadband light emitters. The goal of this proposal is to develop such multi-alloy structures grown by metal-organic vapor phase epitaxy and molecular beam epitaxy for efficient, broadband light emission. To develop broadband emitters we will focus our efforts on this class of fractal and chirped quantum-well structures utilizing InAlGaP alloys grown by metal-organic vapor phase epitaxy on GaAs substrates. The work will concentrate on three areas: materials design and growth, characterization and modelling, and device design and fabrication. The interplay of these three parallel efforts will lead to optimized device structures that emit broadband light with at least 300 meV bandwidth in the green to red regions and a few percent external quantum efficiency. Materials and design parameters will be understood through a wide variety of experimental and theoretical tools. To implement this new class of broadband emitters, we will design, grow and fabricate

light-emitting diode structures, and measure electroluminescence spectra, current-voltage, and light-current characteristics.

Keywords: Broadband Light Emitters, Indium-Aluminum-Gallium-Phosphorus, Fractal Lattice and Chirped Quantum Wells

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

208. ENERGY RELATED APPLICATIONS OF SELECTIVE LINE EMITTERS

\$291,000

DOE Contact: Walter M. Polansky, (301) 903-5995
Auburn University (Space Power Institute) Contact:
M. Frank Rose, (334) 844-5894

Infrared heat sources are used extensively for many processes in industry. From initial work, it appears feasible to develop intense infrared sources based upon electronic transitions in compounds of the rare earths which tend to radiate efficiently at discrete wavelengths rather than a continuum. This work is aimed at conducting the basic and exploratory research that will allow the development of high intensity, discrete frequency infrared sources which are custom tailored to specific industrial processes. The Center for the Rare Earth Elements at the DOE Ames Research Laboratory will be used as the source of information for selection of suitable rare earth elements and compounds with prerequisite emissivity properties. Oxide fibers can be formed by soaking activated carbon fibers in a suitable liquid compound of the rare earth, such as a nitrate of the materials. Since activated carbon fibers can be greater than 70 percent porous, a substantial fraction of the liquid can be absorbed for suitable processing. The composite materials are formed into a paper with minor additions of cellulose using standard paper making technology. Subsequent heating in a reducing atmosphere removes the cellulose and carbon, and forms essentially a pure metallic shell, mimicking the size of the activated carbon precursor. Successful samples will also be characterized for strength, flexibility, and lifetime at temperature. Large area radiators for specific frequencies will be constructed and evaluated with the cooperation of an industrial affiliate.

Keywords: Infrared Energy Delivery Sources, Rare Earth Selective Line Emitters, Industrial Processes

209. PHOTO-INDUCED ELECTRON TRANSFER FROM A CONDUCTING POLYMER TO BUCKMINSTER-FULLERENE: A MOLECULAR APPROACH TO HIGH EFFICIENCY PHOTOVOLTAIC CELLS

\$446,000

DOE Contact: Walter M. Polansky, (301) 903-5995
University of California, Santa Barbara Contact:
Paul Smith, (805) 893-8104

The recently-discovered photoinduced electron transfer, with subpicosecond transfer rate, in composites of a conducting polymer, MEH-PPV, and a molecular acceptor, buckminsterfullerene, C_{60} , opens a new opportunity for photovoltaic research. Since the charge transfer takes place ~1000 times faster than the radiative and/or non-radiative decay of photoexcitations, the quantum efficiency for charge transfer and charge separation is near unity. Photoinduced electron transfer across the donor-acceptor rectifying heterojunction offers potential for solar cell applications, using materials that exhibit a unique combination of properties: electronic and optical properties of semiconductors and metals in combination with the attractive mechanical properties and the processing advantages of polymers. The potential advantages of an all-polymer heterojunction solar cell include low cost, large area, and flexibility. The goal of the proposed research is to build upon this novel molecular approach to photo-induced charge separation and charge transfer, with quantum efficiency approaching unity, and to create a capability to efficiently produce flexible, "plastic" solar cells for large areas.

Keywords: Fullerenes, Photovoltaics, Solar Cells

210. SUPERCONDUCTING BITTER MAGNETS

\$300,000

DOE Contact: Walter M. Polansky, (301) 903-5995
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Leslie Bromberg, (617) 253-6919

A novel process for manufacturing high temperature superconducting magnets, using thick-film superconducting material on structural plates, is described. The technique is similar to that used in constructing Bitter magnets. The superconductor is manufactured in the required shape, avoiding the need to develop ductile wires. The structural metal plate serves as the material as well as the quench protector. A dielectric with high electrical resistivity is placed between the conductor and the metal plate (copper, aluminum, composite materials). This method can be utilized for manufacturing solenoidal, toroidal, saddle, and other types of magnets with both high- T_c and low- T_c superconductors. This project will address issues faced in this type of magnet construction (quench protection, materials compatibility, stability, and cooling). Interaction

with the manufacturers to improve the performance of superconducting materials for this application will be maintained. It is expected that in the final phase of this program, magnets will be constructed and tested. The project is in collaboration with the Plasma Fusion Center at the Massachusetts Institute of Technology and the Superconductivity Technology Center at Los Alamos National Laboratory.

Keywords: Bitter Magnets, Superconductivity

211. BLUE-EMITTING DEVICES BASED ON GALLIUM NITRIDE

\$340,000

DOE Contact: Walter M. Polansky, (301) 903-5995

Lawrence Berkeley Laboratory Contact:

Michael D. Rubin, (510) 486-7124

The purpose of this project is to convert the recent breakthroughs in growth of gallium nitride (GaN) into practical ultraviolet and blue light emitting diodes and lasers. Short-wavelength semiconductor devices based on GaN are needed for many important applications such as energy-efficiency illumination, high-density optical data storage, flat-screen color displays, underwater communications, and high-temperature electronics. One of the principal technical problems that limits device applications has been achieving controllable properties with addition of Mg. It was discovered that good quality material could be readily obtained by a variety of doping methods including ion implantation, diffusion and co-evaporation of Mg. The defect studies which guide the improvements in the growth process will be continued. The technology will be transferred to Hewlett-Packard, where it will be reproduced in a large-scale commercial growth system.

Keywords: Gallium Nitride, Blue-Emitting Devices

212. SOLID STATE MULTI-LAYERED BATTERIES

\$296,000

DOE Contact: Walter M. Polansky, (301) 903-5995

Lawrence Livermore National Laboratory Contact:

Richard M. Bionta, (510) 423-4846

The purpose of this project is to develop thin film solid-electrolyte batteries fabricated by the advanced multilayer sputtering techniques developed for X-ray optics. This technique allows the battery to be constructed *in situ* by depositing the anode, electrolyte, and cathode as distinct layers. Solid-electrolyte batteries have long been attractive because of their shelf-life and compatibility with severe environments. Recently, rechargeable lithium cells that operate at ambient temperature have been developed

based on ionically conducting solid polymer electrolytes. This project will concentrate on the development of thin-film solid-electrolyte cells constructed of lithium based inorganic materials fabricated by multilayer sputtering. The ability of this fabrication technique to discretely layer or compositionally grade thin films provides a unique opportunity to investigate the effect of electrode-electrolyte interface structure on cell performance. Finally, the computer control associated with this fabrication technique will allow the deposition of multiple cells in a bipolar configuration with either series or parallel connection. It is anticipated that this research will directly lead to power sources for modern electronic circuits (i.e., microsensors, memory elements, displays, and timers).

Keywords: Solid State Batteries, Solid Electrolyte Batteries, Multilayer Fabrication

213. PV-POWERED, ELECTROCHROMIC WINDOWS

\$330,000

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National Renewable Energy Laboratory Contact:

David K. Benson, (303) 384-6462

This project will develop a retrofit window treatment for architectural windows. The window treatment will be a combination of thin-film photovoltaic cells and an electrochromic coating, both deposited onto a flexible polymer film. The coated polymer film will be applied to the interior surfaces of existing building windows and used to modulate the solar transmittance into the building thereby providing automatic solar-gain control and daylighting control functions which will reduce heating, cooling, and lighting energy usage in the building. This kind of "smart" window covering has the potential to balance the performance of the window, giving it a net energy benefit. It has been predicted to be able to reduce the cooling power demand of a south-facing window in a climate such as southern California by about 40 percent. At present, an estimated 1-1.5 percent of the total cooling energy need in buildings and 10-30 percent of the peak electric utility power demand is caused by windows amounting to about a 1500 MW increase in electric utility peak electric power demand each year due to new windows at a national operating cost of about \$10 billion. New photovoltaic and electrochromic coating designs and new processes for their deposition onto flexible polymer substrates will be developed in this project.

Keywords: Electrochromic Windows, Smart Windows, PV-Powered Windows

**214. A NOVEL TANDEM HOMOJUNCTION SOLAR CELL:
AN ADVANCED TECHNOLOGY FOR HIGH EFFICIENCY
PHOTOVOLTAICS**

\$322,000

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The semiconductor, ZnSnP(2), meets many criteria for large-scale photovoltaic applications. It is isoelectronic with the III-V alloy InGaP(2), but has the advantage, for photovoltaic applications, of not containing expensive and rare group III elements. In addition, this material does not contain toxic heavy metals such as are found in CdTe and CuInSe(2)/CdS thin film solar cells. The absorption coefficient for this material is also very high. The bandgap of ZnSnP(2) has the additional interesting and useful property of ranging from 1.24 to 1.66 eV, depending on the preparation conditions. There is no *a priori* reason that the electronic properties of these materials cannot be made as good as III-V materials, since very high mobilities were only achieved in III-V's after the development of modern epitaxial growth techniques. State-of-the-art metal-organic molecular beam epitaxy (MOMBE) will be used to grow epitaxial layers of ZnSnP(2) on lattice matched GaAs substrates. When the conditions can be established for preparing a material of a given bandgap, a "tandem homojunction" solar cell will be fabricated by variation of growth conditions in the MOMBE chamber in the appropriate way. This device should show significant efficiency advances over a single material device or tandem heterojunction devices where lattice mismatch produces recombination promoting interface states.

Keywords: Tandem-Homojunction Solar Cell, Photovoltaics, Molecular Beam Epitaxy

OFFICE OF FUSION ENERGY

The mission of the Office of Fusion Energy (OFE) is to develop fusion as an environmentally attractive, commercially viable, and sustainable energy source for the Nation and the world. This mission will be accomplished by parallel activities to develop the science and technology base for fusion, the conduct of large-scale experiments to explore the physics and demonstrate the components of fusion technologies, and the construction and operation of fusion power plants that will culminate in a demonstration power plant.

A significant component of the fusion energy program is the development and validation of the materials required for the fusion systems. Materials must be developed that will meet the unique requirements of fusion, as well as the

standard requirements of a high efficiency, high reliability power generating system. The unique requirements of fusion are the result of the intense neutron environment, dominated by the 14 MeV neutrons characteristic of the deuterium-tritium fusion reaction. For performance, the materials must have slow and predictable degradation of properties in this neutron environment. For safety and environmental considerations, materials must be selected with activation products that neither decay too rapidly (affecting such safety factors as system decay heat) nor too slowly (affecting the waste management concerns for end-of-life system components). Materials that meet these requirements are referred to as "Low Activation Materials." Programs to develop the materials for plasma-facing components, for diagnostic and control systems, for structures in the high neutron flux regions, for the production of tritium in the blanket, and for the superconducting magnets required for confinement are sponsored by OFE.

The fusion program in the United States is conducted with a high degree of international cooperation. Of particular importance is the International Thermonuclear Experimental Reactor (ITER) engineering design activity, conducted in partnership with the European Union, Japan, and the Russian Federation. Approximately half of the materials work sponsored by OFE is in support of the ITER collaboration.

**MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION
OR TESTING**

215. STRUCTURAL MATERIALS DEVELOPMENT

\$1,552,000

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ANL Contact: D. L. Smith (708) 252-4837

This program is directed at the development of advanced, low activation structural materials for application in fusion power system first wall and blankets. Emphasis at ANL is on the development of vanadium-base alloys and on chemical corrosion/compatibility of the structural materials with other system materials. The vanadium alloy development is focused on the V-Cr-Ti system, with the goals of identifying promising candidate compositions, determining the properties of candidate alloys, and evaluating the response to irradiation conditions that simulate anticipated fusion system operation. The compatibility studies include vanadium and other candidate structural materials, and focus on the effects of exposure to projected coolants, especially liquid lithium.

Keywords: Vanadium, Compatibility, Lithium, Irradiation Effects, Alloy Development